



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2017 – 12:58 AM EDT

PDB ID : 5T6M
Title : Structure of the tryptophan synthase b-subunit from *Pyrococcus furiosus* with
b-methyltryptophan non-covalently bound
Authors : Buller, A.R.; van Roye, P.; Arnold, F.H.
Deposited on : unknown
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

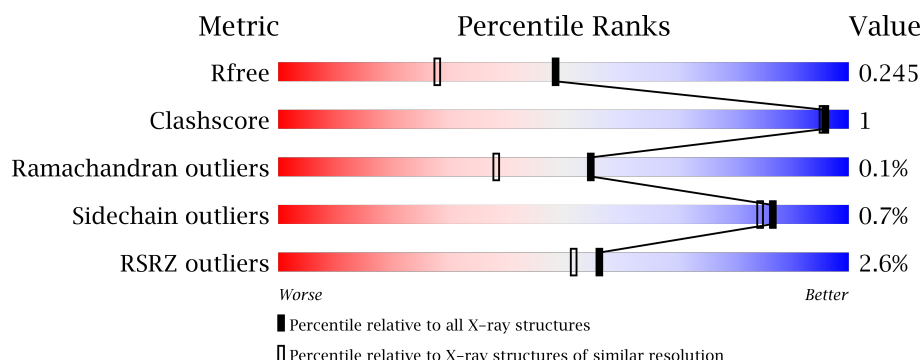
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	396	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 1% 94% 5% </div> </div>
1	B	396	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 1% 93% 5% </div> </div>
1	C	396	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 1%, green 95%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 3% 96% 1% </div> </div>
1	D	396	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 1%, yellow 1%, green 93%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 5% 93% 2% </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NA	D	401	-	-	-	X
4	78U	C	402	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12028 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tryptophan synthase beta chain 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	P	S	0	1	0
			2932	1869	503	547	1	12			
1	B	386	Total	C	N	O	P	S	0	1	0
			2942	1879	506	544	1	12			
1	C	391	Total	C	N	O	P	S	0	0	0
			2967	1892	509	553	1	12			
1	D	382	Total	C	N	O	P	S	0	0	0
			2899	1854	493	539	1	12			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	389	LEU	-	expression tag	UNP Q8U093
A	390	GLU	-	expression tag	UNP Q8U093
A	391	HIS	-	expression tag	UNP Q8U093
A	392	HIS	-	expression tag	UNP Q8U093
A	393	HIS	-	expression tag	UNP Q8U093
A	394	HIS	-	expression tag	UNP Q8U093
A	395	HIS	-	expression tag	UNP Q8U093
A	396	HIS	-	expression tag	UNP Q8U093
B	389	LEU	-	expression tag	UNP Q8U093
B	390	GLU	-	expression tag	UNP Q8U093
B	391	HIS	-	expression tag	UNP Q8U093
B	392	HIS	-	expression tag	UNP Q8U093
B	393	HIS	-	expression tag	UNP Q8U093
B	394	HIS	-	expression tag	UNP Q8U093
B	395	HIS	-	expression tag	UNP Q8U093
B	396	HIS	-	expression tag	UNP Q8U093
C	389	LEU	-	expression tag	UNP Q8U093
C	390	GLU	-	expression tag	UNP Q8U093
C	391	HIS	-	expression tag	UNP Q8U093
C	392	HIS	-	expression tag	UNP Q8U093
C	393	HIS	-	expression tag	UNP Q8U093

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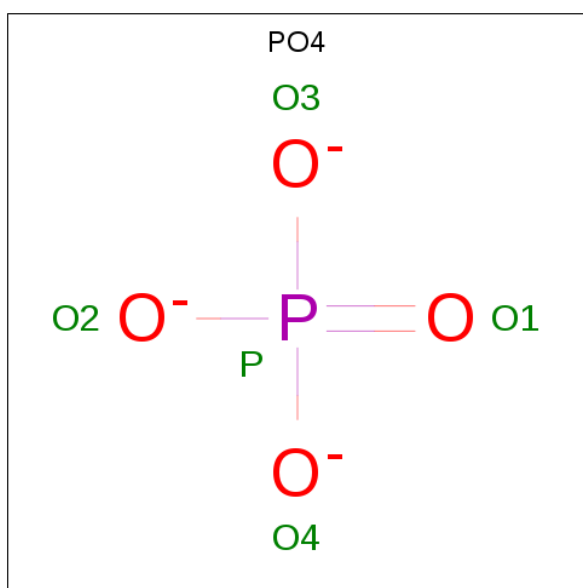
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Chain	Residue	Modelled	Actual	Comment	Reference
C	394	HIS	-	expression tag	UNP Q8U093
C	395	HIS	-	expression tag	UNP Q8U093
C	396	HIS	-	expression tag	UNP Q8U093
D	389	LEU	-	expression tag	UNP Q8U093
D	390	GLU	-	expression tag	UNP Q8U093
D	391	HIS	-	expression tag	UNP Q8U093
D	392	HIS	-	expression tag	UNP Q8U093
D	393	HIS	-	expression tag	UNP Q8U093
D	394	HIS	-	expression tag	UNP Q8U093
D	395	HIS	-	expression tag	UNP Q8U093
D	396	HIS	-	expression tag	UNP Q8U093

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

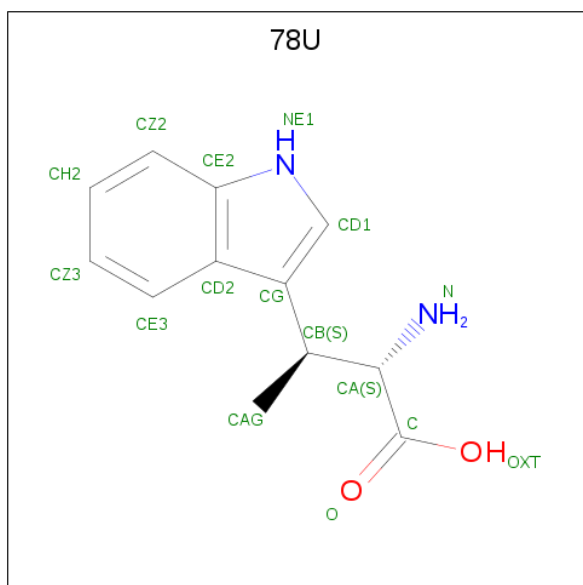
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Na 1 1	0	0
2	A	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0

- Molecule 4 is (betaS)-beta-methyl-L-tryptophan (three-letter code: 78U) (formula: C₁₂H₁₄N₂O₂).

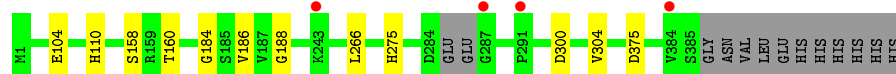


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 16 12 2 2	0	0
4	C	1	Total C N O 16 12 2 2	0	0
4	D	1	Total C N O 16 12 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	70	Total O 70 70	0	2
5	B	54	Total O 54 54	0	0
5	C	49	Total O 49 49	0	0
5	D	53	Total O 53 53	0	0

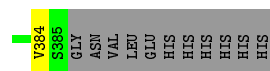
- Molecule 1: Tryptophan synthase beta chain 1



- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| #1 | E73 | V76 | K82 | H110 | D133 | R136 | M139 | K162 | I183 | G184 | I185 | I186 | I187 | G188 | Y192 | Q217 | G229 | V271 | H275 | L278 | I289 | Y301 | F302 | F359 | S385 | G386 | ASN | VAL | LEU | GLU | HIS | HIS | HIS | HIS | HIS | HIS |
|----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- [illegible]

-
- | Topic | Number of Publications |
|-------|------------------------|
| M1 | 1 |
| E17 | 1 |
| F28 | 2 |
| F29 | 2 |
| A47 | 1 |
| D74 | 2 |
| L75 | 2 |
| V76 | 2 |
| H77 | 2 |
| K82 | 1 |
| E132 | 2 |
| G157 | 2 |
| S158 | 2 |
| R159 | 2 |
| N166 | 2 |
| L169 | 1 |
| V173 | 2 |
| A174 | 2 |
| V186 | 2 |
| G216 | 2 |
| L257 | 2 |
| F258 | 2 |
| N267 | 1 |
| F274 | 2 |
| F284 | 2 |
| G1U | 2 |
| G1U | 2 |
| G1Y | 2 |
| Q288 | 2 |
| T289 | 2 |
| K290 | 2 |
| F291 | 2 |
| D300 | 1 |
| R336 | 1 |
| L356 | 1 |
| E359 | 2 |
| N360 | 1 |
| G372 | 2 |



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.82Å 107.70Å 160.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80 38.65 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (40.00-1.80) 99.2 (38.65-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.204 , 0.238 0.211 , 0.245	Depositor DCC
R_{free} test set	6510 reflections (5.20%)	DCC
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12028	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 78U, PO4, LLP, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.53	0/2965	0.59	0/4009
1	B	0.50	0/2981	0.58	0/4034
1	C	0.54	0/3003	0.57	0/4067
1	D	0.53	0/2934	0.56	0/3973
All	All	0.52	0/11883	0.58	0/16083

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2932	0	2900	7	0
1	B	2942	0	2903	12	0
1	C	2967	0	2911	5	1
1	D	2899	0	2839	6	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	5	0	0	0	0
4	B	16	0	0	1	0
4	C	16	0	0	1	0
4	D	16	0	0	1	0
5	A	70	0	0	0	0
5	B	54	0	0	0	0
5	C	49	0	0	0	0
5	D	53	0	0	0	0
All	All	12028	0	11553	30	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (30) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104[A]:GLU:OE1	1:A:104[A]:GLU:N	2.15	0.79
1:B:82:LLP:H4'1	4:B:402:78U:CAG	2.33	0.59
1:B:133:ASP:OD1	1:B:136:ARG:NH2	2.39	0.55
1:B:301:TYR:CD1	1:B:302:PRO:HD2	2.46	0.52
1:B:73:GLU:O	1:B:76:VAL:HG12	2.09	0.51
1:C:82:LLP:H4'1	4:C:402:78U:CAG	2.40	0.51
1:A:158:SER:OG	1:A:160:THR:HG22	2.12	0.50
1:C:110:HIS:CE1	1:C:184:GLY:HA2	2.47	0.50
1:B:183:ILE:HD12	1:B:192:TYR:CD2	2.48	0.49
1:C:73:GLU:O	1:C:76:VAL:HG12	2.14	0.48
1:C:82:LLP:O3	1:C:82:LLP:NZ	2.49	0.45
1:A:104[A]:GLU:CD	1:A:104[A]:GLU:H	2.14	0.45
1:A:110:HIS:CE1	1:A:184:GLY:HA2	2.52	0.45
1:B:271:VAL:CG1	1:B:278:LEU:HD11	2.46	0.45
1:A:188:GLY:HA2	1:A:275:HIS:O	2.18	0.44
1:B:110:HIS:CE1	1:B:184:GLY:HA2	2.52	0.44
1:D:356:LEU:HG	1:D:360:MET:SD	2.58	0.44
1:D:384:VAL:HG12	1:D:384:VAL:O	2.18	0.44
1:B:162:LYS:HD3	1:B:289:ILE:HG21	2.00	0.44
1:B:183:ILE:HD12	1:B:192:TYR:CG	2.52	0.44
1:D:47:ALA:HA	1:D:77:HIS:HB3	2.00	0.43
1:D:169:LEU:HD21	4:D:403:78U:CZ2	2.49	0.43
1:C:237:TYR:HB3	1:C:238:PRO:HD3	2.01	0.43
1:B:82:LLP:O3	1:B:82:LLP:NZ	2.52	0.42
1:A:266:LEU:CD2	1:A:304:VAL:HG11	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:GLY:HA2	1:B:275:HIS:O	2.21	0.41
1:A:266:LEU:HG	1:A:304:VAL:HG11	2.01	0.41
1:B:271:VAL:HG12	1:B:278:LEU:HD11	2.03	0.41
1:D:74:ASP:HB2	1:D:373:ARG:HB3	2.03	0.40
1:D:82:LLP:O3	1:D:82:LLP:NZ	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:SER:OG	1:D:336:ARG:NH1[3_847]	2.07	0.13

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	379/396 (96%)	373 (98%)	5 (1%)	1 (0%)	44	29
1	B	384/396 (97%)	376 (98%)	8 (2%)	0	100	100
1	C	388/396 (98%)	377 (97%)	10 (3%)	1 (0%)	44	29
1	D	377/396 (95%)	370 (98%)	7 (2%)	0	100	100
All	All	1528/1584 (96%)	1496 (98%)	30 (2%)	2 (0%)	55	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	VAL
1	C	186	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	292/315 (93%)	290 (99%)	2 (1%)	87	84
1	B	291/315 (92%)	289 (99%)	2 (1%)	87	84
1	C	293/315 (93%)	291 (99%)	2 (1%)	87	84
1	D	285/315 (90%)	283 (99%)	2 (1%)	87	84
All	All	1161/1260 (92%)	1153 (99%)	8 (1%)	87	84

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	300	ASP
1	A	375	ASP
1	B	139	MET
1	B	217	GLN
1	C	145	LYS
1	C	325	GLU
1	D	267	ASN
1	D	300	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	LLP	A	82	1	24,24,25	2.67	5 (20%)	28,32,34	1.48	7 (25%)
1	LLP	B	82	1	24,24,25	2.48	4 (16%)	28,32,34	1.52	3 (10%)
1	LLP	C	82	1	24,24,25	2.86	5 (20%)	28,32,34	1.47	6 (21%)
1	LLP	D	82	1	24,24,25	2.78	5 (20%)	28,32,34	1.40	3 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	A	82	1	-	0/15/17/19	0/1/1/1
1	LLP	B	82	1	-	0/15/17/19	0/1/1/1
1	LLP	C	82	1	-	0/15/17/19	0/1/1/1
1	LLP	D	82	1	-	0/15/17/19	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	82	LLP	C4-C4'	2.10	1.50	1.46
1	A	82	LLP	C4-C4'	2.32	1.50	1.46
1	D	82	LLP	C4-C4'	2.87	1.51	1.46
1	B	82	LLP	C4-C3	4.15	1.47	1.40
1	C	82	LLP	C4-C3	4.41	1.48	1.40
1	D	82	LLP	C4-C3	4.96	1.48	1.40
1	D	82	LLP	C4-C5	4.99	1.48	1.42
1	B	82	LLP	C4-C5	5.05	1.48	1.42
1	A	82	LLP	C4-C5	5.35	1.48	1.42
1	A	82	LLP	C4-C3	5.36	1.49	1.40
1	D	82	LLP	C4'-NZ	5.53	1.43	1.27
1	A	82	LLP	C4'-NZ	5.54	1.43	1.27
1	C	82	LLP	C4-C5	5.57	1.49	1.42
1	C	82	LLP	C4'-NZ	5.61	1.43	1.27
1	B	82	LLP	C4'-NZ	5.74	1.44	1.27
1	B	82	LLP	C3-C2	7.60	1.46	1.40
1	A	82	LLP	C3-C2	8.10	1.46	1.40
1	D	82	LLP	C3-C2	9.34	1.47	1.40
1	C	82	LLP	C3-C2	9.95	1.47	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	82	LLP	CB-CA-C	-3.77	105.43	111.65
1	B	82	LLP	C4-C3-C2	-3.24	118.16	120.15
1	D	82	LLP	C4-C3-C2	-3.12	118.23	120.15
1	A	82	LLP	C4-C4'-NZ	-2.84	110.88	124.66
1	C	82	LLP	C4-C3-C2	-2.79	118.44	120.15
1	D	82	LLP	C4-C4'-NZ	-2.73	111.41	124.66
1	B	82	LLP	C4-C4'-NZ	-2.68	111.63	124.66
1	A	82	LLP	CB-CA-C	-2.65	107.28	111.65
1	C	82	LLP	C4-C4'-NZ	-2.46	112.72	124.66
1	A	82	LLP	C4-C3-C2	-2.34	118.72	120.15
1	A	82	LLP	C3-C4-C5	-2.09	116.65	118.24
1	C	82	LLP	CD-CG-CB	-2.04	106.38	113.63
1	C	82	LLP	O3-C3-C2	2.04	122.06	117.78
1	C	82	LLP	C6-N1-C2	2.05	123.20	119.26
1	D	82	LLP	C6-N1-C2	2.19	123.47	119.26
1	A	82	LLP	C6-N1-C2	2.23	123.56	119.26
1	A	82	LLP	OP4-C5'-C5	2.55	114.45	109.32
1	A	82	LLP	OP3-P-OP2	2.74	118.68	107.61
1	B	82	LLP	OP4-C5'-C5	3.56	116.49	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	82	LLP	2	0
1	C	82	LLP	2	0
1	D	82	LLP	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	PO4	A	402	-	4,4,4	0.88	0	6,6,6	0.71	0
4	78U	B	402	-	14,17,17	2.50	5 (35%)	13,24,24	1.17	1 (7%)
4	78U	C	402	-	14,17,17	2.55	6 (42%)	13,24,24	1.12	2 (15%)
3	PO4	D	402	-	4,4,4	0.73	0	6,6,6	0.41	0
4	78U	D	403	-	14,17,17	2.58	5 (35%)	13,24,24	0.91	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	A	402	-	-	0/0/0/0	0/0/0/0
4	78U	B	402	-	-	0/5/12/12	0/2/2/2
4	78U	C	402	-	-	0/5/12/12	0/2/2/2
3	PO4	D	402	-	-	0/0/0/0	0/0/0/0
4	78U	D	403	-	-	0/5/12/12	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	403	78U	CG-CD2	-6.15	1.33	1.40
4	C	402	78U	CG-CD2	-4.75	1.35	1.40
4	B	402	78U	CG-CD2	-4.52	1.35	1.40
4	C	402	78U	CZ2-CE2	-4.32	1.34	1.41
4	D	403	78U	CZ2-CE2	-4.16	1.34	1.41
4	B	402	78U	CZ2-CE2	-3.81	1.35	1.41
4	D	403	78U	CE3-CD2	-3.56	1.34	1.42
4	C	402	78U	CE3-CD2	-3.46	1.35	1.42
4	B	402	78U	CE3-CD2	-3.38	1.35	1.42
4	B	402	78U	CD2-CE2	-2.60	1.35	1.42
4	D	403	78U	CD2-CE2	-2.59	1.35	1.42
4	C	402	78U	CD2-CE2	-2.40	1.36	1.42
4	C	402	78U	CD1-NE1	-2.09	1.32	1.36
4	D	403	78U	CG-CB	2.65	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	402	78U	CG-CB	4.44	1.57	1.51
4	B	402	78U	CG-CB	4.78	1.57	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	402	78U	CAG-CB-CA	-3.07	106.85	111.34
4	C	402	78U	CAG-CB-CA	-2.73	107.34	111.34
4	D	403	78U	CE3-CD2-CE2	2.06	120.89	118.17
4	C	402	78U	CAG-CB-CG	2.24	114.44	110.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	402	78U	1	0
4	C	402	78U	1	0
4	D	403	78U	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	382/396 (96%)	-0.09	4 (1%)	82 80	24, 35, 54, 82	0
1	B	385/396 (97%)	0.18	5 (1%)	77 74	24, 38, 55, 67	0
1	C	390/396 (98%)	0.24	11 (2%)	53 48	27, 40, 60, 91	0
1	D	381/396 (96%)	0.37	20 (5%)	28 23	24, 43, 64, 81	0
All	All	1538/1584 (97%)	0.18	40 (2%)	56 52	24, 39, 60, 91	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	291	PRO	4.9
1	D	174	ALA	4.6
1	D	157	GLY	3.9
1	D	166	ASN	3.8
1	D	257	LEU	3.3
1	D	216	GLY	3.3
1	C	257	LEU	3.1
1	D	274	PHE	2.9
1	D	291	PRO	2.9
1	B	385	SER	2.8
1	B	359	GLU	2.8
1	D	284	ASP	2.7
1	A	291	PRO	2.7
1	D	173	VAL	2.6
1	D	258	GLU	2.6
1	D	359	GLU	2.6
1	A	243	LYS	2.5
1	C	176	PHE	2.4
1	D	75	LEU	2.4
1	B	229	GLY	2.4
1	B	186	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	76	VAL	2.4
1	C	239	PHE	2.4
1	A	384	VAL	2.4
1	D	289	ILE	2.4
1	C	315	GLN	2.3
1	A	287	GLY	2.3
1	D	159	ARG	2.3
1	C	285	GLU	2.2
1	C	17	GLU	2.2
1	C	158	SER	2.2
1	D	28	ARG	2.2
1	B	187	VAL	2.2
1	D	17	GLU	2.2
1	D	186	VAL	2.2
1	C	173	VAL	2.1
1	D	132	GLU	2.1
1	D	372	GLY	2.1
1	C	156	SER	2.0
1	D	29	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	LLP	D	82	24/25	0.94	0.16	-	30,32,33,33	0
1	LLP	C	82	24/25	0.96	0.17	-	27,30,30,31	0
1	LLP	B	82	24/25	0.97	0.17	-	24,25,27,27	0
1	LLP	A	82	24/25	0.96	0.14	-	23,26,27,27	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NA	D	401	1/1	0.95	0.26	4.05	44,44,44,44	0
4	78U	C	402	16/16	0.80	0.18	2.41	40,46,50,51	0
4	78U	D	403	16/16	0.91	0.17	1.27	46,48,49,49	0
2	NA	C	401	1/1	0.97	0.11	0.32	37,37,37,37	0
2	NA	B	401	1/1	0.97	0.15	0.26	40,40,40,40	0
4	78U	B	402	16/16	0.94	0.16	0.07	33,34,35,36	0
2	NA	A	401	1/1	0.96	0.11	-0.03	37,37,37,37	0
3	PO4	A	402	5/5	0.97	0.11	-0.42	44,46,49,50	0
3	PO4	D	402	5/5	0.95	0.08	-0.53	54,54,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.